

Tutorial: Reduction of GRI 3.0 mechanism using NLO and SA

Installation

- The Python code of the NLO algorithm is publicly available on GitHub at <https://github.com/IhmeGroup/NLO-Red>
- Dependencies that need to be installed are
 - Python 2.7.x with mpi4py package
 - Cantera with Python interface
 - Ipopt optimization suite
 - Pylpopt python module for calling Ipopt library in Python

Tutorial case

- Reduction of Methane/Air mechanism:
 - Using GRI 3.0 mechanism
 - Qols at atmospheric pressure:
 - Ignition delay of 0-D constant volume reactors with:
 $\phi = \{0.6, 0.7, 0.8, 0.9, 1.0, 1.1, 1.2, 1.3, 1.4\}$
 $T = \{1200, 1400, 1600, 1800\}K$
 - 1-D free-propagating flames with:
 $\phi = \{0.6, 0.7, 0.8, 0.9, 1.0, 1.1, 1.2, 1.3, 1.4\}$
 $T = 300K$

Sensitivity analysis

- **Input file:**
 - Run set-ups
 - verbosity = 'DEBUG' #INFO -- logging verbosity level
 - type_calc = 'SA' -- type of run is SA
 - directory = 'FLAMES' -- directory to store Cantera free flame solutions
 - mechanism = 'gri30.xml' -- chemical mechanism
 - fuel = 'CH4' -- fuel species
 - n2_o2_ratio = 3.76 -- molar ratio of N2 and O2

Sensitivity analysis

- **Input file:**
 - Quantities of Interest
 - Auto-ignition cases
 - $P_{ai} = [1e5]$ -- Initial pressures
 - $T_{ai} = [1200.0, 1400.0, 1600.0, 1800.0]$ -- Initial temperature
 - $\phi_{ai} = [0.6, 0.7, 0.8, 0.9, 1.0, 1.1, 1.2, 1.3, 1.4]$ -- Initial equivalence ratios
 - Free-flame cases
 - $P_{fl} = [1e5]$ -- Pressure conditions
 - $T_{fl} = [300.0]$ -- Temperatures of unburnt mixture
 - $\phi_{fl} = [0.6, 0.7, 0.8, 0.9, 1.0, 1.1, 1.2, 1.3, 1.4]$ -- Equivalence ratios

Sensitivity analysis

- **Results:**

- The case can be run with the command:

`mpirun -np $NP python $NLO_RED_PATH/src/LaunchMPI.py input.py &> log,`

where `$NP` is the number of processes, `$NLO_RED_PATH` is the `NLO_RED` installation directory.

- Two output files will be created:
 - `log`: normal outputs of Cantera and Python
 - `out.log`: logging information of interests, such as sensitivity coefficients and errors as species are removed sequentially

Sensitivity analysis

- Sensitivity coefficients:

```
INF0:root:Task launching and result collection done
INF0:root:HCN 0.0017865585778128544
INF0:root:H2CN 0.0019560865080851917
INF0:root:NNH 0.001980177458335997
INF0:root:N0 0.002020589582128682
INF0:root:N02 0.0021595145487632392
INF0:root:HN0 0.0021749841521168283
INF0:root:NH 0.0022432345158413395
INF0:root:NC0 0.002261347175411166
INF0:root:N20 0.00228368411943832
INF0:root:HNC0 0.00229914236634519
INF0:root:CN 0.0023234725547385485
INF0:root:HCNN 0.002323820835533273
INF0:root:NH3 0.002341654657660448
INF0:root:H0CN 0.002351100316122703
INF0:root:HCN0 0.002353527813810024
INF0:root:CH3CH0 0.0032038013678215215
INF0:root:NH2 0.0035681461966583124
INF0:root:AR 0.004856322420611482
INF0:root:N 0.006604018666539294
INF0:root:C3H7 0.006692428626867639
INF0:root:CH2C0 0.008827863890774851
INF0:root:HCC0 0.010260048315443563
INF0:root:C3H8 0.01057151366652479
```


Sensitivity analysis

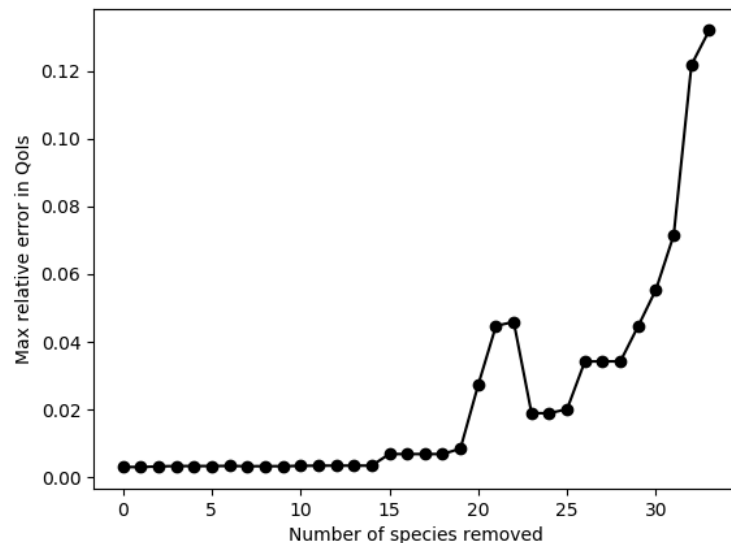
- Removing species sequentially:

```
INF0:root:Last species removed: CH2OH
```

```
INF0:root:Total error with 34 removed species: 0.13196114495425457
```

- After removing 34 species, the flame cases will fail to converge
- The current history of errors as species are removed is listed:

```
INF0:root>Error history: [0.003085555096702663, 0.0030251458744821242, 0.0032433330283269473, 0.0033403596937220887, 0.0033404832526348683, 0.0033474776227780103, 0.0033709387448930847, 0.0032937005049586653, 0.0033020941332582267, 0.0033058602587845948, 0.0033953445201177243, 0.003451278548352368, 0.003464023908518603, 0.0034639182809131984, 0.0034634263283909116, 0.006886429413422369, 0.00687627646259586, 0.006874580270641467, 0.00687504557559089, 0.008485219791336348, 0.02731321266299904, 0.04473009865341194, 0.04587951039780115, 0.01894616868014099, 0.018945678108993492, 0.020127534801022025, 0.0342179109618105, 0.03423374437714729, 0.034244119923574956, 0.04462660409579307, 0.055415071448719135, 0.07148998742755988, 0.12179813266432828, 0.13196114495425457]
```



Non-linear optimization

- **Input file:**
 - Run set-ups
 - verbosity = 'DEBUG' #INFO -- logging verbosity level
 - type_calc = 'OPT' -- type of run is NLO
 - directory = 'FLAMES' -- directory to store Cantera free flame solutions
 - mechanism = 'gri30.xml' -- chemical mechanism
 - fuel = 'CH4' -- fuel species
 - n2_o2_ratio = 3.76 -- molar ratio of N2 and O2

Non-linear optimization

- **Input file:**
 - NLO settings
 - `threshold = 1e-3` -- threshold value of weight β for a species to be discarded
 - `species_exclude_init = (...)` -- species to be removed BEFORE calculating reference Qols
 - `species_exclude_zero = (...)` -- species imposed to be removed and are not in the optimization loop (e.g. inert species, species for NOx mechanism, ...)
 - `species_major = (...)` -- species imposed to be retained and are not in the optimization loop
 - From GRI 3.0 mechanism, 24 species remains to be optimized after specifying `species_exclude_zero` and `species_major` (see the example input file)

Non-linear optimization

- **Input file:**
 - Quantities of Interest
 - Auto-ignition cases
 - $P_{ai} = [1e5]$ -- Initial pressures
 - $T_{ai} = [1200.0, 1400.0, 1600.0, 1800.0]$ -- Initial temperature
 - $\phi_{ai} = [0.6, 0.7, 0.8, 0.9, 1.0, 1.1, 1.2, 1.3, 1.4]$ -- Initial equivalence ratios
 - $tolerance_{ai} = 0.05$ -- relative error tolerance
 - Free-flame cases
 - $P_{fl} = [1e5]$ -- Pressure conditions
 - $T_{fl} = [300.0]$ -- Temperatures of unburnt mixture
 - $\phi_{fl} = [0.6, 0.7, 0.8, 0.9, 1.0, 1.1, 1.2, 1.3, 1.4]$ -- Equivalence ratios
 - $tolerance_{fl} = 0.05$ -- relative error tolerance

Non-linear optimization

- **Results:**

- The case can be run with the command:

`mpirun -np $NP python $NLO_RED_PATH/src/LaunchMPI.py input.py &> log,`

where `$NP` is the number of processes, `$NLO_RED_PATH` is the `NLO_RED` installation directory.

- Two output files will be created:
 - `log`: normal outputs of Cantera, Python, and Ipopt
 - `out.log`: logging information of interests, such as current solution vector and error constraints violation

Non-linear optimization

- Results:

```
INF0:root:Current solution satisfies constraint
INF0:root:Current vector
INF0:root:[ 1.00000001e+00,1.00000001e+00,2.36399390e-01 -9.99520505e-09
-9.99488741e-09,1.00000001e+00,9.11789210e-01,1.00000001e+00
-9.99221123e-09,1.00000001e+00 -9.99379595e-09 -9.99579899e-09
,2.58821355e-02,5.00698225e-02,1.00000001e+00,1.00000001e+00
,9.78139317e-01 -9.99518964e-09 -9.99509732e-09 -9.99497141e-09
-9.99501118e-09 -9.99472493e-09 -9.99555037e-09 -9.99484258e-09]
INF0:root:Number of eliminated species
INF0:root:12
INF0:root:List of eliminated species
INF0:root:C -9.995205052401032e-09
INF0:root:CH -9.99488740774212e-09
INF0:root:CH2OH -9.992211225374772e-09
INF0:root:CH3OH -9.993795945579008e-09
INF0:root:C2H -9.99579898801685e-09
INF0:root:HCCO -9.995189644616228e-09
INF0:root:CH2CO -9.99509731740966e-09
INF0:root:HCCOH -9.99497141262319e-09
INF0:root:C3H7 -9.995011175586161e-09
INF0:root:C3H8 -9.994724932380954e-09
INF0:root:CH2CHO -9.995550368513393e-09
INF0:root:CH3CHO -9.994842582743342e-09
```

Non-linear optimization

- Validation:

- The reduced mechanism created from this tutorial is included at `derived_mechanisms/METHANE/0.05/0.05.cti`

